

OPTICAL STUDY AND SIMULATION OF DIFFUSION  
OF COPPER IONS IN THE  $\text{LiNbO}_3$  CRYSTALSDmytro Sugak<sup>1,2</sup>, Uliana Yakhnevych<sup>1</sup>, Oleh Buryy<sup>1</sup>, Ihor I. Syvorotka<sup>2</sup>, Stepan Hurskyy<sup>1,3</sup><sup>1</sup>Lviv Polytechnic National University, Lviv, Ukraine; <sup>2</sup>Scientific Research Company 'Electron-Carat', Lviv, Ukraine;<sup>3</sup>Institute for Energy Research and Physical Technologies, Goslar, Germany*uliana.v.yakhnevych@lpnu.ua*<https://doi.org/10.23939/jcpee2022>.

**Abstract:** The article deals with research into the processes of diffusion and drift of copper ions in a lithium niobate crystal after annealing in the presence of a copper film deposited on the crystal surface. For this purpose, there are chosen temperatures  $T = 600, 650, 700, 750$  and  $800^\circ\text{C}$ , with the duration of high-temperature annealing being 6 hours for each sample. The optical absorption spectra of the samples are recorded in the direction perpendicular to the direction of diffusion at different distances from the edge of the crystal. Absorption bands of  $\text{Cu}^+$  (400 nm) and  $\text{Cu}^{2+}$  (1000 nm) ions are observed in all the samples annealed. The intensity of the bands varies depending on the annealing temperature and the distance from the diffusion source. Concentrations of copper ions are calculated using the Smakula–Dexter formula. Depth dependences of the Cu ions concentration are approximated within the framework of the model, taking into account both diffusion and drift of Cu ions. Experimental spatial distributions of copper ion concentrations are well approximated by theoretical curves calculated within the framework of the mathematical model of diffusion. The diffusion coefficients determined from the approximations are well-agreed with the available data from the literature.

**Keywords:** lithium niobate; diffusion; drift; optical spectroscopy; impurity concentration.

### 1. Introduction

High-temperature processing of lithium niobate ( $\text{LiNbO}_3$ , LN) in different conditions (oxidizing, reduction and in the presence of metal ions) is an effective method of influencing the state of the defective subsystem of crystals and, accordingly, modifying their optical, electrophysical, and other properties. In particular, annealing in the presence of metal ions that can change their valence under the influence of light and thermochemical treatments (Cu, Fe, Mn, their combinations and combinations with other dopants) is used to increase the photorefractive sensitivity of

$\text{LiNbO}_3$ , which makes it attractive for use in optical information recording devices [1].

In most known works [2, 3], the diffusion of copper ions in LN is studied when the crystals are heated to relatively low temperatures (no more than  $800^\circ\text{C}$ ) in solutions or melts of salts containing Cu, and the depth of its diffusion is determined by the methods of secondary ions mass spectroscopy (SIMS) or Auger spectroscopy. At the same time, the probing radiation spreads along the diffusion direction perpendicular to the surface through which the dopant diffused. The depths that can be investigated using these techniques are no more than 10 microns. The influence of high-temperature and long-term annealing of LN samples with copper films deposited on the surface and samples immersed in copper oxide powder on the optical properties of crystals is studied in papers [4, 5, 6]. However, only in [6] the changes in the absorption spectra caused by copper diffusion with depth (more than 10 mm) along the crystal-physical axes X, Y, Z are studied when the spectra are recorded in the directions perpendicular to the diffusion one. As a result, it was found that the depths of incorporation of copper ions depend on the crystallographic direction, reach values of several hundred microns and are different for  $\text{Cu}^+$  and  $\text{Cu}^{2+}$  ions. The greatest depth of copper penetration is in the Z direction. In this case, the dependence of the distribution of the copper ion concentrations "embedded" in the crystal lattice with depth has a "bell" shape with maxima in the range of  $200\ldots 300\ \mu\text{m}$  from the edge of the plate, depending on the annealing conditions and the charge of the copper ion.

At the same time, the dependence of the depth of incorporation of ions on the annealing temperature, when the source of copper ions is the same for all samples under research, remains unstudied. Also, there is no mathematical description of the dependences of the distribution of copper ions of different valence, which were "embedded" in the crystal lattice of lithium niobate as a result of diffusion processes.

Therefore, the aim of this work is to investigate the distributions of copper ions of different valence diffused to the crystal in the Z direction from the same type of source, depending on the annealing temperature, as well as an attempt to describe mathematically the obtained dependences of the concentration distribution with distance from the sample surfaces.

## 2. Details of the experiment

Crystals of LiNbO<sub>3</sub> of congruent composition were obtained at Scientific Research Company 'Electron-Carat' by the Czochralski method from platinum crucibles in air according to the technology described in [7]. Samples for research were made from one crystal ingot in the form of oriented plates 10×10×2 mm in size (Z, X, Y). The Cu film with a thickness of about 650 nm was deposited on the XY surface of the plates by the magnetron method before thermal treatment. Each sample was annealed at  $T = 600, 650, 700, 750$  and  $800^\circ\text{C}$  for 6 hours. Annealing took place in air in a Nabertherm furnace (Germany). In all cases, the heating rate was  $5^\circ\text{C}$  per minute. After the annealing was completed, the samples were cooled together with the oven.

The absorption spectra after annealing were recorded using a Shimadzu UV-3600 spectrophotometer (Japan) successively in thin layers of the LN sample under study. For this, a movable table with a micrometric screw was located in the sample chamber of the spectrophotometer, which made it possible to move the sample of the investigated crystal, fixed on it, in steps of  $20\text{ }\mu\text{m}$  relative to a fixed diaphragm with a diameter of  $70\text{ }\mu\text{m}$  and a height of  $10\text{ mm}$ . The diaphragm was cut from an opaque ceramic plate and placed parallel to the XY surface of the LN plate and perpendicular to the Z direction (diffusion direction). Scanning was carried out along with the crystal physical direction Z (the diffusion direction), while the scanning light after the slit propagated perpendicular to the chosen crystal-physical direction (diffusion direction). To detect changes in optical properties caused by heat treatment, difference spectra were constructed between the absorption in the central region of the plate and the absorption in each thin layer during scanning. A detailed procedure for measuring spatial changes in the optical absorption of lithium niobate crystals caused by diffusion is given in [8-10].

As mentioned above, the penetration depth of copper is greatest in the crystallographic direction Z [6], so the diffusion of copper was studied in this direction, and the spectra were recorded in the Y direction.

## 3. Study of the diffusion of Cu ions

In the spectra of additional absorption caused by the incorporation of Cu, bands are distinguished with a maximum in the region of  $400\text{--}450\text{ nm}$  and in the

region of  $980\text{--}1000\text{ nm}$ . These bands are typical to LN crystals doped with copper ions – the  $400\text{--}450\text{ nm}$  band is due to the  $\text{Cu}^+ \rightarrow \text{Nb}^{5+}$  intervalence transition, and the band with a maximum of  $980\text{--}1000\text{ nm}$  is due to the  ${}^2\text{E}_g \rightarrow {}^2\text{T}_{2g}$  intracenter transition in the  $\text{Cu}^{2+}$  ion [11-15]. For example, Fig. 1 shows the spectrum of additional absorption obtained at a distance of  $250\text{ }\mu\text{m}$  from the edge of the plate, which was annealed at a temperature of  $800^\circ\text{C}$ .

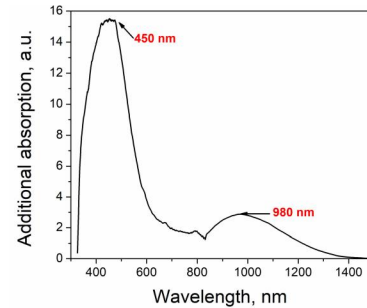


Fig. 1. Additional absorption spectrum obtained at a distance of  $250\text{ }\mu\text{m}$  from the edge of the plate annealed at  $800^\circ\text{C}$ .

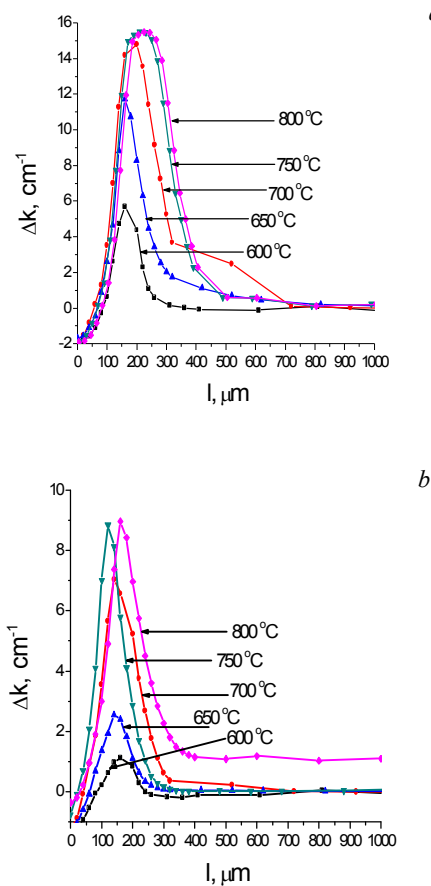


Fig. 2. Depth dependences of the absorption coefficient at wavelengths of  $400\text{ (a)}$  and  $1000\text{ (b)}$  nm, obtained after 6-hour annealing in the presence of a Cu film at  $600, 650, 700, 750$ , and  $800^\circ\text{C}$ .

Dependencies of the change in the absorption value at wavelengths of 400 and 1000 nm with the distance from the edge of the plate for the used annealing temperatures are shown in Fig. 2.

For  $\text{Cu}^{2+}$  ions (1000 nm), the maximum positions of the absorption distribution curves with depth are at a distance of about 180  $\mu\text{m}$  from the edge of the plate. Taking into account the accuracy of the measurements, it can be assumed that the position of the maximum in this case practically does not show any dependence on the annealing temperature. For  $\text{Cu}^+$  ions (400 nm), the maxima of the absorption curves change with temperature and are located at a distance of 150  $\mu\text{m}$  at  $T = 600^\circ\text{C}$  and 250  $\mu\text{m}$  at  $T = 800^\circ\text{C}$ . As can be seen from Fig. 2, with temperature increasing, the intensity of absorption increases and reaches saturation at temperatures of 750...800 $^\circ\text{C}$ , which may be related to the depletion of the diffusion source.

Analysis of the shape of additional absorption bands (Fig. 1), which are caused by  $\text{Cu}^+$  and  $\text{Cu}^{2+}$  ions and obtained at different distances from the edge of the plates, made it possible to calculate the concentration of impurities and estimate their distribution in different crystallographic directions of LN samples, using the Smakula-Dexter formula [16] and data on the magnitudes of the oscillator strengths of the corresponding optical transitions [12, 13]. During the calculations, it was assumed that the shapes of the absorption bands are close to Gaussian, and, accordingly, the expression for the calculations takes the form [16]:

$$N(\text{cm}^{-3}) = 8,7 \cdot 10^{16} \frac{n}{(n^2 + 1)^2} \frac{1}{f_0} K_{\max} \Delta E, \quad (1)$$

where  $n$  is the refractive index at the wavelength of the maximum of the absorption band, which was calculated according to the Zellmeyer formula for  $\text{LiNbO}_3$  [17],  $f_0$  is the oscillator strength of the optical transition, which is  $4 \cdot 10^{-2}$  for the absorption of  $\text{Cu}^+$  (band in the region of 400 nm) and  $2 \cdot 10^{-4}$  for  $\text{Cu}^{2+}$  (band in the region of 1000 nm) [18, 13],  $K_{\max}$  is the absorption coefficient at the maximum of the corresponding band, determined in  $\text{cm}^{-1}$ ,  $\Delta E$  is the width of the corresponding absorption band determined at half its height, in eV.

Concentration distribution curves correspond in shape to absorption distribution curves, however, the concentration of  $\text{Cu}^{2+}$  ions is higher than the concentration of  $\text{Cu}^+$  ions (Fig. 3.). The concentration of  $\text{Cu}^{2+}$  ions in the peaks after high-temperature annealing at the studied temperatures is of the order of  $(0.5...5.5) \cdot 10^{19} \text{ cm}^{-3}$ , and for  $\text{Cu}^+ \sim (1.1...2.5) \cdot 10^{18} \text{ cm}^{-3}$ .

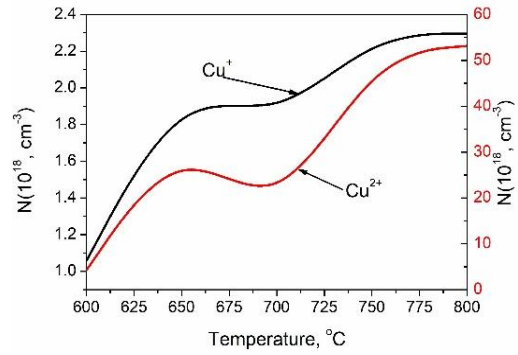


Fig. 3. Distribution curves of  $\text{Cu}^{2+}$  and  $\text{Cu}^+$  ion concentrations

#### 4. Mathematical description of the coloring processes of lithium niobate crystals after high-temperature annealing in the presence of copper ions

As it is known, the electrical conductivity of LN crystals is primarily considered to be ionic and due to the movement of lithium ions [19]. In particular, when transferred along the Z axis of the crystal, they can move through the channels formed by oxygen octahedra. Another possible agent responsible for the electrical conductivity of lithium niobate is oxygen vacancies. Constants in the Arrhenius law for the diffusion coefficient of Li ions in LN [19],

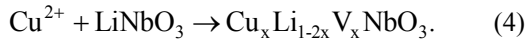
$$D = D_0 \exp\left(-\frac{E}{kT}\right), \quad (2)$$

according to the data of various researchers, differ significantly:  $D_0$  varies from  $1.5 \cdot 10^{-9}$  to  $5.7 \cdot 10^3 \text{ cm}^2/\text{s}$ , diffusion activation energy  $E$  from 0.36 to 3.24 eV. Congruent LN crystals are characterized by non-stoichiometry – an excess of niobium, which partially occupies the positions of lithium. Since the anti-site ion of niobium has an excess positive charge, there is a need for its charge compensation. It is believed [20] that, at least at sufficiently high temperatures, charge compensation is carried out by lithium vacancies, with four lithium vacancies per anti-site niobium ion:

$$[\text{Nb}_{\text{Li}}^{4+}] = 4[V_{\text{Li}}'] \quad (3)$$

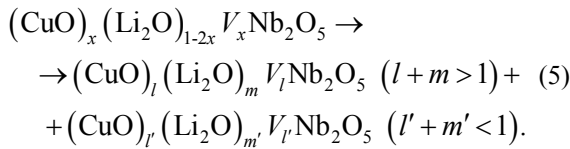
A mathematical model that would describe the process of incorporation metal ions into LN or lithium tantalate in works [2, 3, 21] has not been developed. In general, the presence of a maximum in the distribution of copper is explained by the occurrence of blocking forces in the near-surface layer, which are associated with its structural rearrangement. The authors of [2] present the main processes that, according to their opinion, take place during ion exchange. In particular, when  $\text{Cu}^{2+}$  copper ions are incorporated into the crystal, these processes should be as follows.

1) Formation of compounds with a composition different from the composition of the LN in the near-surface layer:

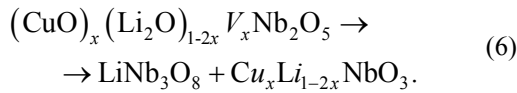


Additional lithium vacancies ( $V_x$ ) arising in accordance with (Eq. 4) carry out charge compensation of copper ions, which, compared to lithium ions, have an additional positive charge.

2) Replacement of  $\text{Li}^+$  with  $\text{Cu}^{2+}$  in the near-surface layer complicates the diffusion of lithium (reduces its diffusion coefficient) due to the creation of barrier layer. This divides the diffusion region into two parts: one enriched with  $\text{Li}_2\text{O} + \text{CuO}$  (lithium niobate-based solid solution), the other depleted by both ion exchange participants:



3) A monoclinic  $\text{LiNb}_3\text{O}_8$  phase appears in the lithium-depleted region:



Obviously, the diffusion coefficient for the exchange mechanism should go down with a decrease in the concentration of exchange participants (since the probability of their falling into neighboring positions in the lattice decreases). Thus, the decrease in the concentration of Li in the near-surface region due to its replacement by Cu and vacancies stops the process of introduction of copper into the crystal due to a decrease in the corresponding diffusion coefficient. The probabilities of the  $\text{Cu}^{2+} \leftrightarrow \text{Li}^+$  exchange process begin to depend on the orientation: movement in the direction away from the crystal surface becomes more probable than movement in the opposite direction. This causes the appearance of a characteristic maximum on the distribution curve of  $\text{Cu}^{2+}$  concentration in the crystal.

The concentration of lithium in the near-surface layers reducing, the possibility of incorporation copper from the surrounding medium (powder or film) to the crystal is practically impossible, so diffusion in this case can be considered as diffusion from a finite source into a semi-infinite body (since the diffusion length  $L$ , which was calculated for the maximum time annealing, is much smaller than the size of the crystal). The mathematical description of the  $\text{Cu}^{2+}$  introduction process will be described in accordance with [22].

Therefore, if the probabilities of jumping diffusant atoms in opposite directions are different, a drift component appears in the diffusion equation:

$$\frac{\partial N}{\partial t} = D \frac{\partial^2 N}{\partial x^2} - V \frac{\partial N}{\partial x}, \quad (7)$$

where  $N$  is the diffusant concentration,  $V$  is the drift velocity. The resulting solution of the diffusion equation for a semi-infinite body with a reflective boundary has the form [8]:

$$N(x, t) = \frac{M}{\sqrt{\pi D t}} \exp\left(-\frac{(x - Vt)^2}{4Dt}\right), \quad (8)$$

where  $M$  is the number of particles per unit area of the source.

Let us use Eq.8 to approximate the dependence of the concentration of  $\text{Cu}^{2+}$  and  $\text{Cu}^+$  ions, which are incorporated into the LN crystal as a result of high-temperature annealing with a deposited copper film. The results of such an approximation are shown in Fig. 4, for clarity, it is given only at a temperature of 800°C. The obtained characteristics of the distributions (position of the maximum  $X_{\max}$ , diffusion coefficient  $D$ , drift velocity  $V$ ) are indicated in Table I.

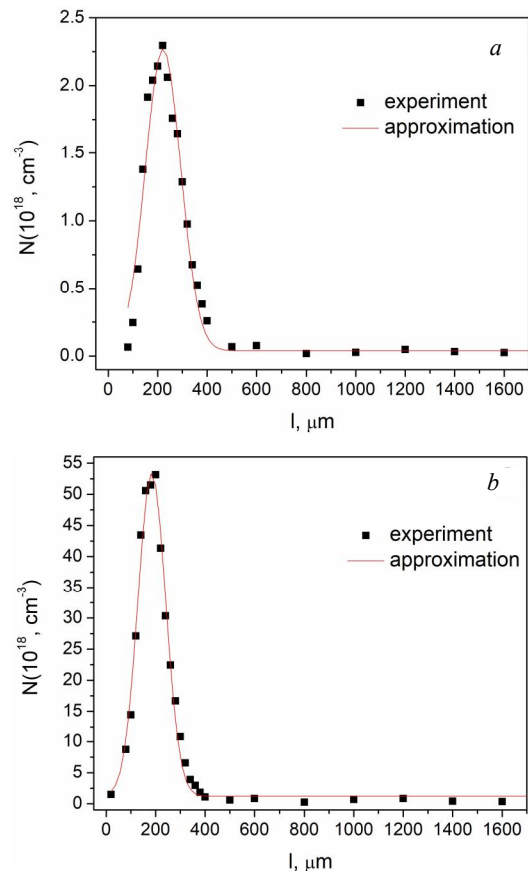


Fig. 4. Distributions of concentrations of  $\text{Cu}^+$  (a) and  $\text{Cu}^{2+}$  (b) ions during diffusion in the Z direction at a temperature of 800 °C and their approximation by Eq. 8.

As can be seen from Fig. 4, Gaussian dependence (Eq.8) generally describes well the concentration distributions of copper ions in the LN crystal. Some inconsistency is connected, first of all, with the not very significant accuracy of determining the dopant concentration according to Eq.1.

Diffusion coefficients determined from the approximations are from  $1.2 \cdot 10^{-10}$  to  $8.4 \cdot 10^{-10}$  cm<sup>2</sup>/s for Cu<sup>+</sup> ions and from  $3.7 \cdot 10^{-10}$  to  $8 \cdot 10^{-10}$  cm<sup>2</sup>/s for Cu<sup>2+</sup> ions depending on the annealing temperature, i.e. in order of magnitude they correspond to the above estimate  $D = 4.1 \cdot 10^{-10}$  cm<sup>2</sup>/s. Drift velocities are from  $1 \cdot 10^{-7}$  to  $\sim 8.4 \cdot 10^{-7}$  cm/s for Cu<sup>+</sup> ions and from  $5.9 \cdot 10^{-7}$  to  $8.5 \cdot 10^{-7}$  cm/s for Cu<sup>2+</sup> ions, respectively.

Table 1

**Parameters of approximation of concentration distributions by a Gaussian dependence in the Z direction**

Ions	$X_{max}, \mu\text{m}$	$D, 10^{-10} \text{ cm}^2/\text{s}$	$V, 10^{-7} \text{ cm/s}$
600°C			
Cu <sup>+</sup>	163±1	3.2±0.2	7.54±0.06
Cu <sup>2+</sup>	140±3	6.2±0.7	6.5±0.1
650°C			
Cu <sup>+</sup>	182±4	8±1	8.4±0.2
Cu <sup>2+</sup>	157±2	8.0±0.5	7.26±0.07
700°C			
Cu <sup>+</sup>	158±3	3.6±0.6	7.3±0.1
Cu <sup>2+</sup>	144±1	5.1±0.3	6.65±0.05
750°C			
Cu <sup>+</sup>	142±2	3.7±0.3	6.55±0.08
Cu <sup>2+</sup>	127±1	4.6±0.3	5.86±0.05
800°C			
Cu <sup>+</sup>	222±3	1.2±0.1	1.0±0.1
Cu <sup>2+</sup>	185±1	7.3±0.4	8.54±0.06

The errors in the determination of the diffusion coefficients and the drift velocities indicated in Table 1 are underestimated, since they do not take into account the error in determining the duration of the annealing process.

## 6. Conclusions

It is shown that the structure of the spatial distribution of copper ions incorporated into a lithium niobate crystal during annealing with a copper film deposited on crystal surface is due to a complex ion exchange process involving copper and lithium ions. In the process of such an exchange, the near-surface layer of the crystal becomes depleted in lithium ions and enriched with copper ions that reduces the exchange diffusion coefficient in this layer. At that the probabilities of jumping copper ions in opposite directions begin to differ, and as a result, the movement of Cu<sup>+</sup> and Cu<sup>2+</sup> ions towards the middle of the crystal becomes predominant. In terms of the transfer process, this is equivalent to the appearance of a drift component in the diffusion equation. The solution of this equation assumes the existence of a maximum in the dependence of the concentration of diffusant ions on the depth, similar to

those observed in our experiments. The approximation of the obtained experimental spatial distributions of Cu<sup>+</sup> and Cu<sup>2+</sup> concentrations during diffusion for different temperatures showed a good agreement with the experiment.

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## ОПТИЧНЕ ДОСЛІДЖЕННЯ ТА МОДЕЛЮВАННЯ ДИФУЗІЇ ІОНІВ МІДІ В КРИСТАЛІ $\text{LiNbO}_3$

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Досліджено процеси дифузії та дрейфу іонів міді в кристалі ніобату літію після відпалу в присутності плівки міді, нанесеної на поверхню кристала. Для дослідження було обрано температури  $T = 600, 650, 700, 750$  та  $800^\circ\text{C}$ , а тривалість високотемпературних відпалів була 6 годин кожний зразок. Спектри оптичного поглинання зразків реєстрували в напрямку, перпендикулярному напрямку дифузії на різних відстанях від краю кристала. Смуги поглинання іонів  $\text{Cu}^+$  (400 нм) і  $\text{Cu}^{2+}$  (1000 нм) спостерігали у всіх відпалених зразках. Інтенсивність смуг змінюється в залежності від температури відпалу та відстані від джерела дифузії. Концентрації іонів міді розраховували за формулою Смакулі–Декстера. Глибинні залежності концентрації іонів  $\text{Cu}$  були апроксимовані в рамках моделі з урахуванням як дифузії, так і дрейфу іонів  $\text{Cu}$ . Експериментально просторові розподіли концентрацій іонів міді добре апроксимуються теоретичними кривими, розрахованими у рамках вказаної математичної моделі дифузії. Визначені з наближень коефіцієнти дифузії добре узгоджуються з відомими з літератури.



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